

N71-15253

**NASA TECHNICAL
MEMORANDUM**

NASA TM X- 52943

NASA TM X- 52943

**AN EFFICIENT METHOD OF
ENERGY PROJECTION**

**CASE FILE
COPY**

by William F. Ford and Richard C. Braley
Lewis Research Center
Cleveland, Ohio

TECHNICAL PAPER proposed for presentation at
Winter Meeting of the American Physical Society
Stanford, California, December 28-31, 1970

AN EFFICIENT METHOD OF ENERGY PROJECTION

by William F. Ford and Richard C. Braley

Lewis Research Center
National Aeronautics and Space Administration
Cleveland, Ohio

ABSTRACT

The standard methods of projecting energy spectra from Hartree-Fock intrinsic wave functions become very time-consuming as the model space is enlarged. One of these methods, however, can be revised so as to minimize storage and handling requirements. A careful description of the technique is presented for the general case, together with sections concerning simplifications resulting from certain nuclear symmetries, and suggestions related to efficiency and accuracy in the actual calculation.

INTRODUCTION

The abundance of experimental information supporting the shell model of the nucleus has made it our most valuable tool for investigating nuclear structure. Shell model calculations become quite complex for deformed nuclei, however, because of the large number of configurations which must be employed. As a result of this, the Hartree-Fock model has in recent years become a very popular substitute for the shell model. In some fashion which is not yet entirely clear, the extra degrees of freedom afforded by the intrinsic Hartree-Fock wave function contrive to produce extrinsic, or physical, states which are in many ways equivalent or superior to shell model states.

One problem associated with the Hartree-Fock model is that physical states must be extracted from the intrinsic wave function by some form of angular momentum projection. When one is dealing only with expectation values of single-particle operators the problem is not too difficult, and has recently been treated in a systematic manner.⁽¹⁻³⁾

To find the energy spectrum of a nucleus, however, one needs the expectation value of a two-particle operator - and the problem is then vastly more complicated.

Four different methods of energy projection are discussed by Ripka.⁽⁴⁾ Of these, the first two are hopelessly impractical for nuclei with more than a few active nucleons. The third method makes use of a complete set of intermediate two-particle two-hole states to evaluate the required matrix elements; simplifications which arise for even-even $N = Z$ nuclei are described in some detail by Tewari and Grillo.⁽⁵⁾ The basic difficulty with this method is that the sum over intermediate states is really a sum over unoccupied orbits, and thus, when the model space is enlarged to reduce truncation error, the number of terms becomes inordinately large.

By making use of closure one may transform the sum over unoccupied orbits into a sum over the occupied orbits, leading to the fourth method mentioned briefly by Ripka. For large model spaces this technique should be the most efficient, if properly applied. A version employed by Gunye and Warke⁽⁶⁾ has the disadvantage that it involves two-body matrix elements depending on the magnetic quantum numbers; the total number of matrix elements which must be handled is thus very large. The version presented here constructs coupled orbital matrix elements from the coupled two-body matrix elements, thus minimizing storage and handling requirements. A complete treatment is given for the most general case, followed by sections describing the simplifications resulting from certain kinds of symmetry. A concluding section suggests some means of improving efficiency and accuracy in the actual calculation.

THEORY

In the axially-symmetric Hartree-Fock model for deformed nuclei, the intrinsic state of a nucleus is represented by a Slater determinant Φ which is an eigenstate of J_z ,

$$J_z \Phi = \hbar K \Phi.$$

but not of J^2 . Physical states of the nucleus must therefore be obtained by means of a projection operator,

$$\begin{aligned}\Psi_{JM} &= P_{MK}^J \Phi \\ &= \frac{2J+1}{2} \int_0^\pi d_{MK}^J(\theta) \tilde{\Phi}(\theta) \sin \theta d\theta,\end{aligned}$$

where $\tilde{\Phi}(\theta) = \exp(-i\theta J_y) \Phi$. By construction, the operator P_{MK}^J picks out that part of a function with angular momentum quantum numbers J and K , and changes it so that its J_z -eigenvalue is $\hbar M$.

An important nuclear property is its energy spectrum, which may be determined by evaluating the matrix element

$$E_J = \left\langle \Phi \left| H P_{KK}^J \right| \Phi \right\rangle,$$

or more generally,

$$H_J = \left\langle \Phi' \left| H P_{K'K}^J \right| \Phi \right\rangle,$$

where Φ' is another (possibly identical) Slater determinant.

As is often the case, a straightforward approach proves to be the most efficient in the final analysis. To begin with we have

$$H_J = \frac{2J+1}{2} \int_0^\pi d_{K'K}^J(\theta) H(\theta) \sin \theta d\theta,$$

where

$$\begin{aligned}H(\theta) &= \langle \Phi' | H | \tilde{\Phi} \rangle \\ &= \left\langle \Phi' \left| \left(\sum_{i=1}^A T_i + \frac{1}{2} \sum_{i \neq j}^A V_{ij} \right) \right| \tilde{\Phi} \right\rangle \\ &= T(\theta) + V(\theta).\end{aligned}$$

Now the function Φ may be expanded in either of the forms

$$\begin{aligned}\Phi(12 \dots A) &= A^{-1/2} \sum_{N_a}^A |N_a\rangle \Phi_{N_a}(23 \dots A) \\ &= [2A(A-1)]^{-1/2} \sum_{N_a N_b}^A |N_a N_b\rangle \Phi_{N_a N_b}(34 \dots A),\end{aligned}$$

where $|N_a\rangle$ is a single-nucleon orbital function with the properties

$$J_z |N_a\rangle = \hbar m_a |N_a\rangle,$$

$$\langle N_b | N_a \rangle = \delta_{N_a N_b},$$

and $|N_a N_b\rangle$ is a normalized, antisymmetric orbital pair function:

$$|N_a N_b\rangle = \frac{1}{\sqrt{2}} (|N_a\rangle |N_b\rangle - |N_b\rangle |N_a\rangle).$$

Using these expansions we obtain

$$\begin{aligned}T(\theta) &= \sum_{N'_a N_a} \langle N'_a | T | \tilde{N}_a \rangle \langle \Phi'_{N'_a} | \tilde{\Phi}_{N_a} \rangle \\ V(\theta) &= \frac{1}{4} \sum_{N'_a N_b} \sum_{N'_a N'_b} \langle N'_a N'_b | V | \tilde{N}_a \tilde{N}_b \rangle \langle \Phi'_{N'_a N'_b} | \tilde{\Phi}_{N_a N_b} \rangle,\end{aligned}$$

where the rotated orbitals $|\tilde{N}_a\rangle$ are defined by

$$|\tilde{N}_a\rangle = e^{-i\theta J_y} |N_a\rangle.$$

Let us now indicate explicitly the dependence of the various matrix elements on the rotation angle θ . We begin with the identity

$$|N_a\rangle = \sum_{JM} P_{MM}^J |N_a\rangle,$$

from which it follows that

$$|\tilde{N}_a\rangle = \sum_{JMM'} d_{M'M}^J(\theta) P_{M'M}^J |N_a\rangle.$$

A similar relation holds for the orbital-pair state $|\tilde{N}_a \tilde{N}_b\rangle$, and in both cases the inner sum over M reduces to one term because the operand states are eigenfunctions of J_z . The orbital kinetic energy matrix element thus becomes

$$\begin{aligned} \langle N'_a | T | \tilde{N}_a \rangle &= \sum_J d_{m'_a m_a}^J(\theta) \left\langle N'_a \left| T \left(\sum_{M'M} P_{M'M}^J \right) \right| N_a \right\rangle \\ &= \sum_J d_{m'_a m_a}^J(\theta) \langle N'_a | T_J | N_a \rangle, \end{aligned}$$

and, with a similar abbreviation,

$$\langle N'_a N'_b | V | \tilde{N}_a \tilde{N}_b \rangle = \sum_J d_{M'_{ab} M_{ab}}^J(\theta) \langle N'_a N'_b | V_J | N_a N_b \rangle,$$

where $M_{ab} = m_a + m_b$ and $M'_{ab} = m'_a + m'_b$. We refer to $\langle N'_a | T_J | N_a \rangle$ and $\langle N'_a N'_b | V_J | N_a N_b \rangle$ as coupled orbital matrix elements.

The angular dependence of the various overlap integrals cannot be displayed so explicitly. It turns out, however, that they are all proportional to the overlap integral

$$\Delta(\theta) = \langle \Phi' | \tilde{\Phi}(\theta) \rangle$$

which is a very sharply peaked function of its argument. This dependence may be factored out by defining the one- and two-nucleon density matrices

$$\begin{aligned}\left\langle \Phi'_{N'_a} \left| \tilde{\Phi}_{N_a} \right. \right\rangle &= \Delta(\theta) \langle N'_a | \rho^{(1)} | N_a \rangle \\ \left\langle \Phi'_{N'_a N'_b} \left| \tilde{\Phi}_{N_a N_b} \right. \right\rangle &= \Delta(\theta) \langle N'_a N'_b | \rho^{(2)} | N_a N_b \rangle,\end{aligned}$$

in terms of which

$$H(\theta) = \Delta(\theta)h(\theta),$$

$$h(\theta) = t(\theta) + v(\theta),$$

$$t(\theta) = \sum_{N'_a N_a} \sum_J d_{m'_a m_a}^J(\theta) \langle N'_a | T_J | N_a \rangle \langle N'_a | \rho^{(1)} | N_a \rangle,$$

$$v(\theta) = \frac{1}{4} \sum_{N_a N_b} \sum_{N'_a N'_b} \sum_J d_{M'_{ab} M_{ab}}^J(\theta) \langle N'_a N'_b | V_J | N_a N_b \rangle \langle N'_a N'_b | \rho^{(2)} | N_a N_b \rangle.$$

The matrices $\rho^{(1)}$ and $\rho^{(2)}$ are angle-dependent, but weakly so, and satisfy the relationship

$$\begin{aligned}\langle N'_a N'_b | \rho^{(2)} | N_a N_b \rangle &= \langle N'_a | \rho^{(1)} | N_a \rangle \langle N'_b | \rho^{(1)} | N_b \rangle \\ &\quad - \langle N'_a | \rho^{(1)} | N_b \rangle \langle N'_b | \rho^{(1)} | N_a \rangle.\end{aligned}$$

The one-nucleon density matrix $\rho^{(1)}$ is numerically equal to the transpose inverse of the matrix G whose elements are

$$\langle N'_a | G | N_a \rangle = \left\langle N'_a \left| e^{-i\theta J_y} \right| N_a \right\rangle = \sum_J d_{m'_a m_a}^J(\theta) \langle N'_a | G_J | N_a \rangle,$$

$$\langle N'_a | G_J | N_a \rangle = \left\langle N'_a \left| \sum_{M'M} P_{M'M}^J \right| N_a \right\rangle,$$

and one may further show that $\Delta(\theta) = \det \{ \langle N'_a | G | N_a \rangle \}$.

Next we turn to the question of isotopic spin. The single-nucleon orbitals will be assumed to be eigenstates of the z-component of the isotopic spin operator, so that

$$|N_a\rangle = |n_a\rangle |\tau_a\rangle.$$

The kinetic energy integrand $t(\theta)$ will therefore divide into two parts, $t_p(\theta)$ and $t_n(\theta)$. The first consists of all those terms in $t(\theta)$ for which both N'_a and N_a refer to proton orbits; the second consists of the remaining terms, for which both N'_a and N_a refer to neutron orbits. There are no cross terms.

The potential energy integrand $v(\theta)$ divides into three parts, $v_p(\theta)$, $v_n(\theta)$, and $v_{pn}(\theta)$. The first consists of those terms in $v(\theta)$ for which all four labels refer to proton orbits; the second consists of those terms for which all four labels refer to neutron orbits. The third part $v_{pn}(\theta)$ consists of the remaining terms in $v(\theta)$, which involve only orbital pairs in which one nucleon is a proton and the other is a neutron.

Using symmetry arguments one may restrict the summation for $v_{pn}(\theta)$ so that N'_a and N_a refer to proton orbits and N'_b and N_b to neutron orbits, provided the result is multiplied by four. Similar arguments allow one to restrict the summation for $v_p(\theta)$ and $v_n(\theta)$ so that $n_b < n_a$ and $n'_b < n'_a$, again provided that the result is multiplied by four.

It is convenient to introduce an isospin projection operator $P_{\mu\mu}^T$, and use the identity

$$V = V \left(\sum_{T\mu\mu'} P_{\mu\mu'}^T \right).$$

for this allows part of the dependence of the coupled orbital matrix elements on the labels τ_a, τ_b to be isolated:

$$\langle N'_a N'_b | V_J | N_a N_b \rangle = \sum_{T=0} A_T(\tau_a \tau_b) \langle N'_a N'_b | V_J | N_a N_b \rangle_T.$$

The isospin-coupled orbital pair state $|N_a N_b\rangle_T$ is defined by

$$|N_a N_b\rangle_T = \frac{1}{\sqrt{2}} \left(|n_a\rangle |n_b\rangle + (-1)^T |n_b\rangle |n_a\rangle \right) \chi_T,$$

χ_T being a singlet or triplet isospin function, and the coefficient $A_T(\tau_a \tau_b)$ has the value δ_{T1} for the integrands $v_p(\theta)$ and $v_n(\theta)$ and the value $1/2$ for the integrand $v_{pn}(\theta)$.

Finally we consider the question of parity. It is generally assumed that each single-nucleon orbital $|N_a\rangle$ is an eigenfunction of the parity operator with eigenvalue π_a ; this permits further restrictions on the summations. In particular, the orbital pairs (N_a, N_b) needed to evaluate $v(\theta)$ can be classified as shown in Table I:

TABLE I. - (N_a, N_b) ORBITAL
PAIR ORDERING

Integrand	Pair restrictions		
	Isospin	Parity	Other
$v_p(\theta)$	(p, p)	(+, +)	$n_b < n_a$
		(-, -)	$n_b < n_a$
		(+, -)	
$v_n(\theta)$	(n, n)	(+, +)	$n_b < n_a$
		(-, -)	$n_b < n_a$
		(+, -)	
$v_{pn}(\theta)$	(p, n)	(+, +)	
		(-, -)	
		(+, -)	
		(-, +)	

BASIS FUNCTIONS

The most general solution of the Hartree-Fock equations would, of course, yield the exact radial and angular dependence of all the orbital functions. Usually the complexities of this task are avoided by assuming that each orbital function is accurately described by an expansion

$$|N_a\rangle = \sum_k C_k(N_a) |km_a\rangle |\tau_a\rangle$$

in terms of a limited number of orthonormal (single-particle) basis functions $|km_a\rangle$ which are eigenfunctions of j_z with eigenvalue $\hbar m_a$, eigenfunctions of the parity operator with eigenvalue π_a , and are otherwise labeled by the index k . When the basis functions are also individually eigenfunctions of j^2 they are said to form a spherical basis; this is the only kind considered here. We assume that the simplified Hartree-Fock equations have been solved and that the coefficients $C_k(N_a)$ are known.

The elements of the matrix G_J , from which $\rho^{(1)}$, $\rho^{(2)}$, and Δ are eventually to be constructed, may now be written

$$\langle N'_a | G_J | N_a \rangle = \delta_{\tau'_a \tau_a} \delta_{\pi'_a \pi_a} \sum_{k_1} D_{k_1}(N'_a) C_{k_1}(N_a) \delta_{j_1 J}.$$

The coefficients $D_k(N'_a)$ are the analogues of $C_k(N_a)$ for the final-state orbitals $|N'_a\rangle$, which we assume are also described by the same set of basis functions $\{|km_a\rangle\}$. The kinetic energy matrix elements are similar in structure, having the form

$$\langle N'_a | T_J | N_a \rangle = \delta_{\tau'_a \tau_a} \delta_{\pi'_a \pi_a} \sum_{k_1 k_2} D_{k_2}(N'_a) \langle k_2 || T || k_1 \rangle C_{k_1}(N_a) \delta_{j_1 j_2} \delta_{j_2 J},$$

$\langle k_2 || T || k_1 \rangle$ being the reduced matrix element (which for the rotationally invariant kinetic energy operator is numerically equal to $\langle k_2 m | T | k_1 m \rangle$ for any m).

To evaluate the potential energy matrix elements, we introduce basis-pair states coupled to good J and T ,

$$|k_1 k_2\rangle_{JT}^{(M)} = \sum_{m_1 m_2} \langle j_1 m_1, j_2 m_2 | JM \rangle |k_1 m_1 k_2 m_2\rangle_T$$

in terms of which

$$|n_a n_b\rangle_T = \sum_{k_1 k_2} C_{k_1}^{(N_a)} C_{k_2}^{(N_b)} \sum_{JM} \langle j_1 m_a, j_2 m_b | JM \rangle |k_1 k_2\rangle_{JT}^{(M)}.$$

The exchange symmetries of the coupled basis-pair states and the Clebsch-Gordon coefficients permit this to be written in the abbreviated form

$$|n_a n_b\rangle_T = \sum_{k_2 \leq k_1} \sum_J C_{k_1 k_2}^{(N_a N_b)} |k_1 k_2\rangle_{JT}^{(M_{ab})},$$

where the coupled coefficients $C_{k_1 k_2}^{JT(N_a N_b)}$ are defined by

$$C_{k_1 k_2}^{JT(N_a N_b)} = C_{k_1}^{(N_a)} C_{k_2}^{(N_b)} \langle j_1 m_a, j_2 m_b | JM_{ab} \rangle + (-1)^T C_{k_1}^{(N_b)} C_{k_2}^{(N_a)} \langle j_1 m_b, j_2 m_a | JM_{ab} \rangle$$

with the proviso that only the first term shall be used when $k_1 = k_2$ and $T = 0$. The coupled orbital potential energy matrix elements may now be expressed quite simply as

$$\left\langle N'_a N'_b | V_J | N_a N_b \right\rangle_T = \sum_{k_2 \leq k_1} \sum_{k_4 \leq k_3} D_{k_3 k_4}^{JT} (N'_a N'_b) C_{k_1 k_2}^{JT} (N_a N_b) \left\langle k_3 k_4 || V || k_1 k_2 \right\rangle_{JT},$$

where $\left\langle k_3 k_4 || V || k_1 k_2 \right\rangle_{JT}$ are the conventional two-body coupled matrix elements.

NEUTRON-PROTON SYMMETRY

For nuclei with $N = Z$, it is common to assume that Φ has n-p symmetry; that is, for each neutron orbital $|n_a\rangle | \tau_a \rangle$ in Φ there is a corresponding proton orbital $|n_a\rangle | -\tau_a \rangle$ identical except for isotopic spin (and similarly for Φ'). The functions $|n_a\rangle$ do not depend on τ_a in this case, and hence the kinetic energy integrand may be written

$$t(\theta) = 2 \sum_{n'_a n_a}^{A/2} \sum_J d_{m'_a m_a}^J(\theta) \langle n'_a | T_J | n_a \rangle \langle n'_a | \rho^{(1)} | n_a \rangle.$$

Now, in general, when it occurs in $v_{pn}(\theta)$ the two-nucleon density matrix has only one term,

$$\langle N'_a N'_b | \rho^{(2)} | N_a N_b \rangle = \langle N'_a | \rho^{(1)} | N_a \rangle \langle N'_b | \rho^{(1)} | N_b \rangle,$$

whereas in $v_p(\theta)$ and $v_n(\theta)$ both of its terms contribute. By rearranging the terms in the series, however, it is possible in the case of n-p symmetry to express the potential energy integrand in terms of the isospin-coupled density matrices

$$\begin{aligned} \left\langle n'_a n'_b | \rho^{(2)} | n_a n_b \right\rangle_T &\equiv \langle n'_a | \rho^{(1)} | n_a \rangle \langle n'_b | \rho^{(1)} | n_b \rangle \\ &+ (-1)^T \langle n'_a | \rho^{(1)} | n_b \rangle \langle n'_b | \rho^{(1)} | n_a \rangle, \end{aligned}$$

which are defined with the proviso that when $n_a = n_b$ and $T = 0$, only the first term is to be used. The final result is

$$v(\theta) = \sum_{n_b \leq n_a}^{A/2} \sum_{n'_b \leq n'_a}^{A/2} \sum_J d_{M'_{ab} M_{ab}}^J(\theta) \times \sum_{T=0}^1 (1 + 2\delta_{T1}) \left\langle n'_a n'_b \right| V_J \left| n_a n_b \right\rangle_T \left\langle n'_a n'_b \right| \rho^{(2)} \left| n_a n_b \right\rangle_T.$$

$R_y(\pi)$ SYMMETRY

The operator which rotates the z-axis through an angle θ about the y-axis is given by

$$R_y(\theta) = e^{-i\theta J_y}.$$

The special case $\theta = \pi$ is important, for the spherical basis functions transform in a particularly simple way when $R_y(\pi)$ is applied:

$$R_y(\pi) |km\rangle = (-1)^{j-m} |k-m\rangle.$$

In general, the orbitals $|N_a\rangle$ do not possess corresponding properties. However, for nuclei with even Z and even N , it is often assumed that Φ itself has $R_y(\pi)$ symmetry; that is, for each orbital $|N_a\rangle$ in Φ there is a corresponding orbital $|\bar{N}_a\rangle$ which satisfies

$$|\bar{N}_a\rangle = R_y(\pi) |N_a\rangle \quad |N_a\rangle = -R_y(\pi) |\bar{N}_a\rangle.$$

As a result, the expansion of Φ may be written

$$\begin{aligned}
\Phi &= A^{-1/2} \left\{ \sum_{N_a}^{A/2} |N_a\rangle \Phi_{N_a} + \sum_{\bar{N}_a}^{A/2} |\bar{N}_a\rangle \Phi_{\bar{N}_a} \right\} \\
&= \left[1 + R_y(\pi) \right] A^{-1/2} \sum_{N_a}^{A/2} |N_a\rangle \Phi_{N_a} \\
&= \left[1 + R_y(\pi) \right] \Phi_1 = \Phi_1 + \Phi_2
\end{aligned}$$

where, for convenience, we specify the subgroup $\{|N_a\rangle\}$ of orbitals which serve to define Φ_1 by the requirement that $m_a > 0$ for each member $|N_a\rangle$. Clearly $\Phi_2 = R_y(\pi)\Phi_1$, and one may also show that $\Phi_1 = R_y(\pi)\Phi_2$ and $\Phi_2 = [R_y(\pi)]^{-1}\Phi_1$. The "rotated" state function $\tilde{\Phi}$ then becomes

$$\begin{aligned}
\Phi(\theta) &= \tilde{\Phi}_1(\theta) + e^{-i\theta J_y} e^{+i\pi J_y} \Phi_1 \\
&= \tilde{\Phi}_1(\theta) + \tilde{\Phi}_1(\theta - \pi),
\end{aligned}$$

and, from the symmetry properties of the reduced rotation matrices,

$$\langle JM | \tilde{\Phi}(\theta) \rangle = \langle JM | \tilde{\Phi}_1(\theta) \rangle + (-1)^{M-K} \langle JM | \tilde{\Phi}_1(\pi - \theta) \rangle.$$

Consequently the integrand $H(\theta)$ may be written

$$H(\theta) = \langle \Phi' | H | \tilde{\Phi}_1(\theta) \rangle + (-1)^{K'-K} \langle \Phi' | H | \tilde{\Phi}_1(\pi - \theta) \rangle,$$

and, if Φ' also possesses $R_y(\pi)$ symmetry,

$$H(\theta) = 2 \left\{ \langle \Phi'_1 | H | \tilde{\Phi}_1(\theta) \rangle + (-1)^{K'-K} \langle \Phi'_1 | H | \tilde{\Phi}_1(\pi - \theta) \rangle \right\}.$$

In either case $H(\theta)$ is of the form $H_1(\theta) + (-1)^{K-K'} H_1(\pi - \theta)$, and by a change of variable in the second term one may obtain

$$H_J = \frac{2J+1}{2} \int_0^\pi H_1(\theta) \left[d_{K,K}^J(\theta) + (-1)^{J-K} d_{K,K}^J(\theta) \right] \sin \theta d\theta.$$

Since the quantum numbers m_a from $|N_a\rangle$ and $|\bar{N}_a\rangle$ will cancel in pairs to give $K = 0$ (regardless of the symmetry assumed for Φ'), this reduces to

$$H_J = 2 \left(\frac{2J+1}{2} \right) \int_0^\pi H_1(\theta) d_{K,0}^J(\theta) \sin \theta d\theta,$$

$$J = 0, 2, 4, \dots$$

For the evaluation of $V(\theta)$ it is convenient to employ a different specification of the manner in which Φ is split into two functions $\Phi_1 = R_y(\pi)\Phi_2$ and $\Phi_2 = R_y(\pi)\Phi_1$. This is accomplished by considering the expansion

$$\Phi = \left\{ 1 + R_y(\pi) \right\} \left[2A(A-1) \right]^{-1/2} \sum_{N_a N_b}^{A/2} |N_a N_b\rangle \Phi_{N_a N_b}$$

and defining the subgroup $\{|N_a N_b\rangle\}$ by the requirement that $M_{ab} > 0$ or $M_{ab} = 0$ and $m_a > 0$. In this way only the rotation matrices $d_{MM'}^J(\theta)$ for $M, M' \geq 0$ need be calculated.

MISCELLANEOUS DETAILS

By far the most time-consuming part of the calculation is the construction of first the coupled coefficients $C_{k_1 k_2}^{JT}(N_a N_b)$ and then the coupled matrix elements $\langle N'_a N'_b | V_J | N_a N_b \rangle_T$. This task is further complicated by

the necessity of keeping track of all the indices in an efficient manner.

Probably the best approach is to order the orbital pairs ($N_a N_b$) first by isospin, then by parity, and last by M_{ab} . (Note that for a given J , only those pairs with $|M_{ab}| \leq J$ will contribute.) The basis pairs may be ordered in a somewhat similar fashion: first by parity, and then by J (such that $|j_1 - j_2| \leq J \leq j_1 + j_2$). Thus the pairs are arranged in the order in which they will be needed, and can be located by a single incrementing index.

Much time can be saved if the Clebsch-Gordan coefficients are calculated in advance, stored, and retrieved as needed. Ordinarily this requires some testing of the angular momentum quantum numbers to avoid dealing with those coefficients which automatically vanish. This testing is time-consuming, however, and it may prove to be more efficient in the final analysis to dispense with it entirely and simply multiply by the zero coefficient. The storage and retrieval problem can also be simplified if zero coefficients do not have to be avoided. Whatever the choice, it is worthwhile to check that $\min(j_1, j_2) \geq \min(|m_a|, |m_b|)$, as these quantities can be calculated in advance when the pairs are ordered and later referenced by the same incrementing indices.

Once the coupled matrix elements have been obtained, the integrands $t(\theta)$ and $v(\theta)$ are computed for selected angles by summing over the initial-and final-state orbitals. In the usual case where $\Phi' = \Phi$, one can substantially shorten the calculation by making the replacements

$$\sum_{N'_a N_a} \rightarrow 2 \sum_{N'_a \leq N_a} \epsilon(N'_a, N_a)$$

$$\sum_{N'_a N'_b} \sum_{N_a N_b} \rightarrow 2 \sum_{N'_a N'_b \leq N_a N_b} \epsilon(N'_a N'_b, N_a N_b)$$

where $\epsilon(\alpha, \beta) = 1 - \frac{1}{2} \delta_{\alpha\beta}$. Any suitable algorithm may be used for the numerical integration, but of course Gaussian quadrature is an obvious choice. It should be noted, however, that $\Delta(\theta)$ is a very sharply peaked function, so that some care must be taken in order to insure sufficient accuracy. In a typical calculation for ^{20}Ne , for instance, $\Delta(\theta)$ falls from 1.0 at $\theta = 0^\circ$ to 0.07 at $\theta = 45^\circ$ to 0.001 at $\theta = 65^\circ$. In contrast, $h(\theta)$ varies relatively slowly over the entire angular range, changing by less than 50 percent. Probably the most satisfactory method of dealing with such an integrand is to base the Gaussian quadrature on polynomials orthogonal with respect to a weight function similar to $\Delta(\theta)$, but this is an involved procedure. Fortunately the zeroes of the Legendre polynomials are concentrated at the ends of the angular range, and this feature may be further enhanced by an appropriate change of integration variable before the quadrature method is applied.

REFERENCES

1. W. F. Ford and R. C. Braley, NASA TN D-5879.
2. R. C. Braley and W. F. Ford, Phys. Rev. 182, 1174 (1969).
3. W. F. Ford and R. C. Braley, To be published in Nuclear Physics.
4. G. Ripka, Lectures in Theoretical Physics, Vol. VIIC (University of Colorado Press, 1965), pp. 237-298.
5. S. N. Tewari and D. Grillot, Phys. Rev. 177, 1717 (1969).
6. M. R. Gunye and C. S. Warke, Phys. Rev. 156, 1087 (1967).